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### NATIONAL BUREAU OF STANDARDS

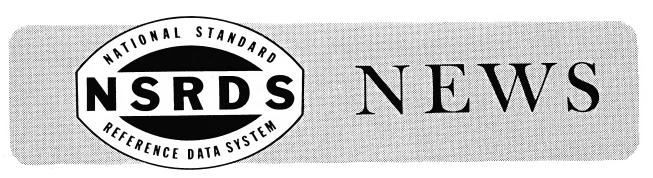
# **Technical News Bulletin**

REPRINT



UNITED STATES DEPARTMENT OF COMMERCE The TECHNICAL NEWS BULLETIN is published monthly to keep science and industry informed regarding the technical programs, accomplishments, and activities of the National Bureau of Standards. The Bureau is organized as follows: Institute for Basic Standards, Institute for Materials Research, Institute for Applied Technology, Center for Radiation Research, and Center for Computer Sciences and Technology.

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The NSRDS was established to make critically evaluated data in the physical sciences available to science and technology on a national basis. The NSRDS is administered and coordinated by the NBS Office of Standard Reference Data.

APPROACH OF CHEMICAL
THERMODYNAMICS DATA CENTER
TO FORMULA DESIGNATIONS OF
CHEMICAL COMPOUNDS

The Chemical Thermodynamics Data Center, under the direction of D. D. Wagman, National Bureau of Standards, U.S. Department of Commerce prepares an annual index of the published literature on measurements of a number of thermodynamic and related properties (enthalpy, entropy and heat capacity at 298.15 K, and the enthalpy of formation at 0 K) of chemical substances and mixed systems. The index is published as part of the annual Bulletin of Thermodynamics and Thermochemistry, under the sponsorship of the Commission on and Ther-Thermodynamics mochemistry of the International Union of Pure and Applied Chemistry (IUPAC). For this index the Chemical Thermodynamics Data Center based its order of listing on the system used in its compilations of Selected Values of Chemical Thermodynamic Properties, NBS Circular 500\* and the NBS Technical Note 270\*\* series¹ (SD Catalog numbers C13.46:270-3; C13.46:270-

\*Out of Print

4, \$1.25 each; and C13.46:270-5, 55 cents). This system, which covers pure substances and aqueous solutions, gives a uniquely specified location for each substance independent of the manner in which the chemical formula is written or how the substance is named, but keeps together those species that are closely related chemically. It is based on the system originally described by E. W. Washburn in the International Critical Tables, Vol. I, p. 96, and has been modified and simplified to include the new synthetic elements and their compounds. It has been further extended to incorporate provisions for allovs and other mixtures and solutions.

The elements are arranged in the "spread" formation of the Periodic Table and are assigned consecutive "finding numbers," starting with oxygen, next hydrogen, and proceeding down each group of the Table and moving from right to left. The order of the elements and their finding numbers are shown in the accompanying illustration.

The location of any compound is determined by the "finding formula," the set of finding numbers of the elements that constitute the compound. Each substance is located in a table corresponding to the largest finding number in the finding formula. Within each table compounds are arranged in the order of increasing finding number for the other elements. The hydrogen and oxygen due to water of hydration in hydrated salts are

not included in the finding formula; hydrates are located immediately after the anhydrous salt. The following sequence of finding numbers illustrates the general principle of the order of arrangement (tables are separated by semicolons):

1; 2,2-1; 3.3-1,3-2,3-2-1; 4,4-1,4-2,4-2-1,4-3,4-3-1,4-3-2,4-3-2-1; etc.

Metal alloy systems and other mixtures and solutions are treated somewhat differently, for the convenience of the users of the Index. Alloy systems, as distinguished from intermetallic compounds, are written with a slash between each of the elements making up the system. They are entered in the tables for each of the elements of the alloy. Within each table the alloy is entered immediately after the pure element, in ascending order of the finding numbers of the remaining elements. Intermetallic compounds, on the other hand, are treated as ordinary compounds and are indexed only in the table corresponding to the highest finding number in the finding formula.

Mixtures and nonaqueous multicomponent solutions are designated with dashes between the component substances. These systems are indexed in the appropriate positions in the various tables corresponding to each of these component substances.

All sorting and ordering of compounds and systems according to the above rules is presently being done by computer, using programs written by W. H. Evans of the Data Center. These programs are

<sup>\*\*</sup>Updated Revisions of NBS Circular 500

designed to interpret chemical formulae and reactions, written in upper and lower case letters and with superscripts and subscripts, that have been converted into the General Purpose Scientific Document Image Code developed at NBS.\*\*\*

The elements in the chemical formula for a substance as entered into the computer may be written in any order; the computer determines the proper finding numbers and finding formula and orders the substances as described above. The final order Index as printed by the computer contains the original formulae as they were entered. No attempt has been made to rewrite the chemical formulae of compounds or mixed systems in a format corresponding to the Standard Order, since the multiple index entries make this additional refinement unnecessary.

#### BIBLIOGRAPHY ON PROPERTIES OF DEFECT CENTERS IN ALKALI HALIDES

NBS-OSRDB-71-1, Bibliography on Properties of Defect Centers in Alkali Halides<sup>1</sup> (COM-71-00248. Microfiche 95 cents, Hard Copy \$3) by S. C. Jain, S. A. Khan, H. K. Sehgal, V. K. Garg and R. K. Jain is the latest publication of the NBS Office of Standard Reference Data series of bibliographies. References to optical, magnetic, and transport properties of defect centers for impurities and selected molecular ion impurities are surveyed. The defect properties of pure alkali halides are also included. Twenty-five journals were scanned to produce the 3000 references presented in two sections. The first section covers references for the years 1927-1963 inclusively. The second section covers the years from 1964 to the present and is more comprehensive in scope.

## FOUR TRANSLATIONS OF DATA COMPILATIONS FROM THE U.S.S.R.

Four translations of compilations of thermophysical properties data have been published for the U.S. Department of Commerce and the National Science Foundation and are being made available through the National Technical Information Service. A limited number of copies of each translation are also available on request from Information Services, Office of Standard Reference Data, National Bureau of Standards, Washington, D.C. 20234.

Thermophysical Properties of Freon-22 by A. V. Kletskii<sup>1</sup> (\$3, publication from the U.S.S.R. Committee of Standards, Measures and Measuring Instruments, apparently in the series initiated by GSSD (State Service for Standard and Reference Data).

In this book an analysis is made of Soviet and non-Soviet studies on the thermodynamic and physical properties of freon-22, which is one of the most widely used refrigerants. A table is given of the thermodynamic properties of superheated freon-22 vapor in the range -100 to +250 °C, at pressures of 0.02-65 bar (1 bar =  $1 \times 10^5$  N/m<sup>2</sup>). Tables and thermal diagrams are given of the thermodynamic properties of the gas in a state of saturation (from -105 °C to the critical point). Data on the thermal conductivity, viscosity, surface tension. and dielectric properties of freon-22 are analyzed and tabulated.

This book will be useful for engineers and technicians working in the field of refrigeration, and for research workers and students of thermal physics. The book has 20 tables, 7 figures, 2 diagrams, and 69 bibliographical references.

Thermophysical Properties of Air and Air Components<sup>1</sup> by A. A. Vasserman, Ya. Z. Kazavchinskii, and V. A. Rabinovich and edited by A. M. Zhuravlev (\$3, publication

number TT70-50095) describes a method for deriving equations of state from elementary functions conforming to experimental thermodynamic data. The equations of state constructed by this method are sufficiently reliable for computing the thermal and thermodynamic values. A critical analysis is given of the available data on the thermal properties of air, nitrogen, oxygen, and argon. The equations of state for these gases are determined, and detailed tables of their thermodynamic properties are compiled for conditions ranging from the saturation curve to temperatures of 1300 K and pressures of 1000 bar. T-s and i-s diagrams are given for each gas. The experimental data on the viscosity and thermal conductivity of air and its components are analyzed and generalized, and equations are given for computing these properties over a wide range of parameters.

Heavy Water, Thermophysical Properties¹ by Ya. Z. Kazavchinskii et. al. and edited by V. A. Kirillin (\$3, publication number TT70-50094) contains a review, a critical analysis, and a synopsis of most of the papers published on the thermophysical properties of heavy water. This material served to derive equations of state for heavy water and its vapor. These equations form the basis of the comprehensive tables given in the book on thermodynamic properties of heavy water for pressures of up to 500 kg/cm<sup>2</sup> and a temperature range between 3.8 and 550 °C.

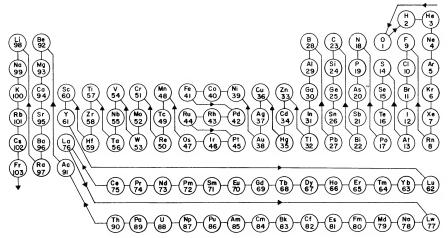
Thermodynamic and Thermophysical Properties of Helium¹ by N. V. Tsederberg, V. N. Popov, and N. A. Morozova and edited by A. F. Alyab'ev (\$3, publication number TT70-50096) contains thermodynamic and thermophysical properties of helium in the ranges of pressure from 0.2 to 200 bar and of temperature from 0 to 3000 °C. An equation of state for helium is given, and the thermal properties are cal-

<sup>\*\*\*</sup>See NSRDS News April 1968 and NSRDS News February 1970.

culated. By means of the rules of statistical thermodynamics, the authors calculated the specific heat, enthalpy, and entropy of helium in the perfect gas state. The influence of the real state of the gas on the thermodynamic properties was estimated from the equation of state for helium. The i-s diagram was constructed and equations were formulated for describing the thermal conductivity and the viscosity of helium in given temperature and pressure ranges.

#### TABLES OF DIELECTRIC CONSTANTS, DIPOLE MOMENTS, AND DIELECTRIC RELAXATION TIMES

The Office of Standard Reference Data has available a limited number of reprints of Tables of Dielectric Constants, Dipole Moments and Dielectric Relaxation Times compiled by Worth E. Vaughan of the University of Wisconsin. These Tables are a reprint from the 1969 issue of the Digest of Literature on Dielectrics published by the National Academy of Sciences.



Standard Order of Arrangement of the Elements. Compounds are located in the Table for the element (in the compound) having the highest number in the above figure.

The Tables contain unevaluated data reported in publications abstracted by *Chemical Abstracts* for 1969. In most cases the values cited have been taken from the original literature. In cases where the original literature was unavailable, the *Chemical Abstracts* citation follows the reference. The Tables cover measurements on pure materials and dilute solutions but do not include work in mixtures or poorly characterized substances.

The following tables are given:

- 1. Static Dielectric Constants of Pure Liquids
- 2. Static Dielectric Constants of Pure Solids
- 3. Dipole Moments
- 4. Unresolved Relaxation Times
- 5. Resolved Relaxation Times

Copies may be obtained from: Information Services, Office of Standard Reference Data, National Bureau of Standards, Washington, D.C. 20234.

<sup>1</sup> Order by number from the National Technical Information Service, Springfield, Va. 22151, for the price indicated.